INFRARED SPECTRA OF ANIONIC COBALT-CARBON DIOXIDE CLUSTERS

BENJAMIN KNURR, J. MATHIAS WEBER, *Department of Chemistry and Biochemistry, JILA - University of Colorado, Boulder, CO, USA*.

We present infrared photodissociation spectra of $Co(CO_2)_n^-$ ions (n = 3 – 11) in the wavenumber region 1000 – 2400 cm^{-1}, interpreted with the aid of density functional theory calculations. The spectra show signatures of several structural motifs for the interaction of a Co atom and CO_2 ligands. The spectra are dominated by a core ion showing bidentate interaction of two CO_2 ligands forming C-Co and O-Co bonds. The prevalence of triplet vs singlet states and the charge distribution in the $Co(CO_2)_2^-$ core ion will also be discussed.